A Short Introduction to EMCUR

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INTRODUCTION

The Monte Carlo (MC) technique, as is used in carrier transport calculations in semiconductors, is a general tool for device modeling and simulation. Like any numerical simulator, the art of simulation is to simplify the design process, to determine ultimate performance limits for a given technology, and to provide physical insights into the device/phenomena under investigation. One of the major advantages of the MC method over other conventional analytic/numerical techniques is its greater ability to handle realistic band and scattering details without assuming a priori the distribution functions. Hence, it is especially useful in modeling submicron devices in which hot-carrier effects as well as time- and space-dependent phenomena are dominant.

EMCUR (Ensemble Monte Carlo at the University of Rochester) is a general-purpose software package for simulating III-V compound devices with variable band parameters. This version (1R3K) of the program is a one-dimensional (1D in r space) simulator which is suitable for simulating non-steady-state transport processes in bulk materials, bipolar-type devices, relaxation of photogenerated carriers, etc. Emphasis in the implementation have been placed on user flexibility and variety of available data.

This memo briefly outlines the major features available in EMCUR. For more detailed information on the physical models and numerical algorithms used as well as how to use the program, the reader is referred to the references listed at the end of this memo.

MAJOR FEATURES

General

- It employs the piece-wise constant GAMMA approach to self-scattering approximation, with "fast self-scattering" technique and an "adaptive" maximum electron energy in each valley for the selection of the scattering mechanisms; it also automatically disables the use of piece-wise constant GAMMA approach when the total scattering rate is not a simple monotonic

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increasing function of energy.
- o It has incorporated a self-consistent Poisson solver and a self-consistent screening model which, if invoked, calculate the local potential, field, charge density, and the scattering rates (through the screening length) using the evolving distribution functions in a self-consistent way.
- o It has a user-optional background electron sub-ensemble superimposed on the photoinjected carrier sub-ensemble, which calculates the transport properties of each separate sub-ensemble as well as their combined properties.
- o It has user-enabled/disabled individual scattering mechanisms as well as statistics in each separate valley.
- o It has a "continuous-run mode" (as opposed to the "single-run mode") in which the program takes the state of the ensemble from the previous run as its input, so that the time axis can be expended without losing temporal resolution.
- o It has its own portable pseudorandom number (PRN) generator, which provides machine-independent, uniformly distributed PRN's in (0,1).
- o It is basically an EMC simulator, but it can also be operated in the one-particle MC mode by specifying an ensemble size of 1, and simulating for sufficient long times.

Band and Material Models

- o It uses a three-valley conduction band including nonparabolicity for any III-V ternary compound material (default is AlGaAs) with variable band structures.
- o It handles structures with the following position-dependent parameters:
  - Alloy composition: which can be arbitrarily specified by the user;
  - Band parameters: (temperature-dependent) band gaps, effective masses, nonparabolic parameters, and user-specified conduction-band offset in each valley;
  - Material parameters: high- and low-frequency dielectric constants, crystal density, velocity of sound, deformation potentials, and phonon energies.

  (Note: All of the above parameters can be overridden by user-supplied parameters.)
- o It assumes a flat valence band (infinitely large hole effective masses) when photogenerated electron-hole pairs are injected, and the holes are assumed to be immobile when the net-charge densities are determined by the Poisson solver.

Scattering Mechanisms

- o Phonon scatterings:
  - Intervalley phonon scattering;
  - Intravalley phonon scattering;
  - Polar optical phonon scattering, with or without (self-consistent) screening;
  - Acoustic phonon scattering with deformation-potential interaction;
- o Defect scattering:
  - Ionized impurity scattering;
- o Electron-electron scattering.

Simulation Variables

- o It allows user-specified arbitrary doping and field profiles versus position; also arbitrary time dependence of the applied field and/or bias voltage.

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o It provides user-adjustable meshes of all histograms of interests as well as the time and space axis.
o It allows user-specified (sub-)ensemble size(s), simulation time with three observation times, device length, and lattice temperature.

Initial Conditions

o k space: (five alternatives)
  - Maxwellian distribution (heated or unheated, with user-specified Te; drifted or undrifted, with user-specified vd);
  - Hemi-Maxwellian distribution, i.e., one with only positive velocity component along a given direction (cold or hot, with or without drift);
  - Velocity-weighted Maxwellian distribution (cold or hot, with or without drift);
  - Gaussian (in energy) distribution (with user-specified excitation energy and the width of the laser pulse);
  - "delta-function" (in momentum and energy) distribution (Px=Py=0; Pz=Po, where Po corresponds to some user-specified injection energy with a finite width).
    (Note: Initial valley occupancy for the ensemble can be randomly assigned according to the user-specified initial valley occupancy probability.)
o r space: (four alternatives)
  - delta-function distribution at z=0 or some user-specified "injection plane" inside the device;
  - Uniform distribution;
  - Exponentially decaying function distribution (with user-specified penetration depth and injection level);
  - Arbitrary user-defined distribution.
o Time domain: (four alternatives)
  - delta-function, i.e., the entire ensemble is launched at time t=0;
  - Rectangular pulse (with user-specified pulse width);
  - Gaussian pulse (with user-specified standard deviation);
  - Inverse hyperbolic cosine function (with user-specified FWHM width).
    (Note: The program can handle variable ensemble size to model the injection of a laser pulse.)

Boundary Conditions

o Particle:
  - Perfect absorbing boundary condition (for simulating ohmic contacts or other absorbing boundaries);
  - Periodic boundary condition (for simulating infinite bulk materials);
  - Tunneling boundary condition (for simulating heterostructure hot-electron diodes/transistors).
o Poisson solver:
  - Fixed voltage at both boundaries (with user-specified boundary voltages);
  - Fixed voltage at one boundary and fixed field at the other boundary (with user-specified boundary voltage and field).
    (Note: A user-defined arbitrary depletion charge inside the device can also be specified.)

Histograms and Estimators

o It provides distribution histograms of interests (in each valley separately as well as in all valleys combined) sampled at the initial, three intermediate, and the final times:
  - Velocity, energy, and spatial distributions with user-adjustable range

(the energy histogram is adaptive);
- Average velocity and energy versus distance distributions;
- Potential, field, electron/net-charge concentration profiles inside the device as calculated by the Poisson solver;
- Scattering pattern (i.e., number of scatterings due to each mechanism) as a function of distance;
- Inverse screening lengths versus distance as calculated using the self-consistent screening model;
- Total scattering rate in each valley as a function of energy, which is updated at each time-step when the self-consistent screening model and/or electron-electron scattering are enabled.

o It provides temporal evolution of the kinematic quantities of interests (in each valley separately as well as in all valleys combined):
- Average velocity and energy as well as band occupancy for (separate sub-ensembles and) the total ensemble;
- Mean of ensemble displacement as well as mean of velocity and energy distributions;
- Average scattering angles (ionized impurity, optical phonon, and acoustic phonon scatterings);
- Average mean free times and mean free paths;
- Scattering rates due to each mechanism;
- Current densities (including emission and tunneling currents if tunneling boundary condition is specified);
- Boundary voltages (potential across the device) as calculated by the Poisson solver;
- Maximum total scattering rates which are used for the piece-wise constant GAMMA approach;
- Trajectory of the state of the first electron in the ensemble (valley index, position, velocity, and energy).

Program Outputs

o It provides user-enabled/disabled output data files (all of the above) for post-graphical processing.
o It has user-enabled/disabled plots of the average velocity, energy, and valley occupancy versus time on a line printer for quick inspection.
o It generates a data file which contains the state of the ensemble for the subsequent run in the continuous-run mode;
o It outputs a file which contains information about the current run, e.g., scattering mechanism summary, total number of times to invoke the PRN generator which can be used as a reference for checking the reproducibility, and CPU times, etc.

FOR MORE INFORMATION

This memo only presents an outline of the major features of the EMCUR program. For detailed information on the physical models, numerical algorithms, and device models used in EMCUR, the reader is referred to Ref. [1], EMCUR--An Ensemble Monte Carlo Program for III-V Compound Semiconductor Device Modeling and Simulation, as well as Ref. [2], EMCUR User's Manual, on how to use the program and examples of typical outputs produced by EMCUR. Some earlier documentations about EMCUR and some simulation results are listed in Refs. [3]-[8]. Recent applications to the study of photogenerated carrier transport in GaAs surface space-charge fields and hot-carrier relaxation and scattering processes in bulk GaAs can be found in Refs. [9] and [10], respectively.

REFERENCES

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